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A FORTRAN III (IBM 7090) PROGRAM FOR THE CALCULATION OF ELECTRON WAVE FUNCTIONS FOR THE SODIUM ION

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UNITED STATES NAVAL ORDNANCE LABORATORY, WHITE OAK, MARYLAND

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A FORTRAN III (IBM 7090) PROGRAM FOR THE CALCULATION OF ELECTRON WAVE FUNCTIONS FOR THE SODIUM ION

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ABSTRACT: An IBM 7090 program is described. It calculates, using simplified Hartree-Fock equations, the radial parts of the wave functions for the electrons in the sodium ion. Up to 1000 values for each wave function can be calculated. A complete listing of the subroutines and an example is included in this report.

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A FORTRAN III (IBM 7090) PROGRAM FOR THE CALCULATION OF ELECTRON WAVE FUNCTIONS FOR THE SODIUM ION

This report describes a FORTRAN III (IBM 7090) program for the calculation of sodium-ion wave functions. This has been done in view of future, theoretical evaluations, like transition probabilities and cross sections, which are needed for guidance and interpretation of sodium-arc-tunnel investigations.

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CONTENTS

A FORTRAN III (IBM 7090) PROGRAM FOR THE CALCULATION OF ELECTRON WAVE FUNCTIONS FOR THE SODIUM ION

PURPOSE: **Determination of the radial part of the wave functions for the electrons in the 1-s, 2-s and 2-p shells of the sodium ion. The Hartree-Fock equations are used for this in a simplified form, so that one deals with three uncoupled eigenvalue equations. The theory and the application of the results will be discussed in NOLTR 63-32.**

METHOD:

A. Mathematical

The following equations are solved for the eigenvalues $\varepsilon_1, \varepsilon_2, \varepsilon_3$ and the eigenfunctions $P(1,r)$, $P(2,r)$, $P(3,r)$:

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}[y(r)+y_o(1,1,r)] - \varepsilon_1\right\} P(1,r) = 0$$

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}[y(r)+y_o(2,2,r)] - \varepsilon_2\right\} P(2,r) = 0$$

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}[y(r)+y_o(3,3,r) + \frac{2}{5}\, y_2(3,3,r)] - \varepsilon_3 - \frac{2}{r^2}\right\} P(3,r) = 0$$

where $y(r) = 11 - 2y_o(1,1,r) - 2y_o(2,2,r) - 6y_o(3,3,r)$

and $y_k(n,m,r) = \int_o^r (\frac{\rho}{r})^k P(n,\rho)P(m,\rho)d\rho + \int_r^\infty (\frac{r}{\rho})^{k+1} P(n,\rho)P(m,\rho)d\rho$

with the boundary conditions:

$r \to 0$ $\quad P(1,r) \sim r \quad P(2,r) \sim r \quad P(3,r) \sim r^2$

$r \to \infty$ $\quad P(n,r) \sim e^{-\varepsilon_n \cdot r}$

and the normalization condition $\int_o^\infty P^2(n,\rho)d\rho = 1$

The solutions are obtained by iteration: Starting with a first guess for $\varepsilon_1, \varepsilon_2, \varepsilon_3$ and $P(1,r), P(2,r), P(3,r)$

1) $y(r)$ and $y_k(n,m,r)$ are calculated

2) Then new $P(n,r)$ are calculated by integrating the differential equations from $r = 0$ outwards. This is repeated adjusting ε_n until the absolute value of $P(n,r)$ is a minimum at an arbitrarily chosen, fixed, large r-value. The changes in ε_n are effected as long as they are larger than the required eigenvalue accuracy TE.

3) With the new eigenvalues $\varepsilon_1, \varepsilon_2, \varepsilon_3$ and the pertaining new eigenfunctions $P(1,r)$, $P(2,r)$ $P(3,r)$ the calculations are started again in 1).
This is repeated until $\int_0^\infty (P_{old}-P_{new})^2 dr \leq TT$, the prescribed wavefunction accuracy.

Numerical Remarks:

1) Since the differential equations do not contain the first derivative, Numerov's integration procedure is used: If the D.E. is $f''(r) = a(r) \cdot f(r) + b(r)$ one can, using $\delta^2 f_j = (\Delta r)^2 [f''_j + \frac{1}{12}\delta^2 f''_j]$ and $f_{j+1} = 2f_j - f_{j-1} + \delta^2 f_j$, derive

$$f_{j+1} = \frac{f_j\left[2+ \frac{(\Delta r)^2}{12} \cdot 10 \cdot a_j\right] + f_{j-1}\left[-1 + \frac{(\Delta r)^2}{12} a_{j-1}\right] + \frac{(\Delta r)^2}{12}\left[10\, b_j + b_{j+1} + b_{j-1}\right]}{1 - \frac{(\Delta r)^2}{12} a_{j+1}}$$

2) The preceding formula shows that the numerical procedure is simplified if the values of the independent variable r are equidistant. On the other hand the accuracy is better if $\frac{\Delta r}{r} =$ constant. Therefore as a compromise the r-range is subdivided into several sets and in each of these sets, the r-values are equidistant.

3) Since the eigenvalues can be determined numerically only within a certain accuracy, the pertaining wave functions do not decrease exponentially for increasing r, but their absolute values go through a minimum and increase then exponentially. Therefore the final wave functions are obtained by integrating the differential equations, using the final eigenvalues ε_n, from r = 0 outward and from large r-values inward. The outward and the inward solutions are then matched at some point, which can be prescribed.

4) Since P(3,r) enters in y(r) with the coefficient 6, P(1,r) and P(2,r) however only with the coefficient r , the iteration procedure is speeded up by determining first P(3,r).

B. Programming

Input: in the following order

1) JF

Format (I3), restriction JF $\leq$ 20 , 1 card

JF is the number of sets into which the range of the independent variable r is divided. Each of these sets is once more subdivided into equally spaced intervals. The endpoints of these intervals are the values of r used in the program and calculated by the program in the subroutine Radius.

2) NF(J) XF(J)

Format (I4, E14.6), restriction: NF(JS(L)) $\geq$ 6 , J = 1,...JF,JF cards

NF(J) is the number of intervals into which the Jth set is subdivided.

XF(J) is the right endpoint of the Jth set

3) JS(L)

Format (3I3), L = 1,...3 , 1 card

JS(L) is the number of the r-set in which the backward and the forward integrated solution for the Lth wave function will be matched.

4) TE TT E(1) E(2) E(3)

Format (5E14.6) 1 card

TE is permissible absolute error for eigenvalues.

TT is permissible sum of squared deviations of wave functions .

E(L) is the (guess of the) Lth eigenvalue.

5) P(L,N)

Format (3E14.6), L = 1,...3, N = 1,...NFF

Restriction NFF $\leq$ 1000 , NFF cards

P(L,N) is the Nth value of the guessed Lth wave function.

NFF is the total number of R-points and will be calculated in Radius.

6) DATE

Format (2A5) 1 card

Output: in the following order

1) Each time the calculated eigenvalue E(L) differs from the previous value of E(L) by an amount smaller than TE there will be printed:

a) P(L,N) PB(N)

Format (2E18.9) , N = 1,NFF

P(L,N) is the Nth value of the Lth wave function obtained by forward integration.

PB(N) is the Nth value of the Lth wave function obtained by backward integration.

b) E(L)

Format (E18.9)

E(L) the calculated Lth eigenvalue

2) At the end of the complete calculation will be printed:

a) DATE

Format (2A5)

b) E(L)

Format (3E14.9), L = 1,3

E(L) the final values of the eigenvalues

c) TE, TT

Format (2E14.6)

TE is the permissible absolute error for eigenvalues

TT is the permissible sum of squared deviation of wave functions.

d) R(N) P(1,N) P(2,N) P(3,N) Z(N) ZNL(1,N) ZNL(2,N) ZNL(3,N)

Format (8E14.6), N = 1,NFF

R(N) is the Nth value of the independent variable r

P(L,N) is the Nth value of the final Lth wave function

Z(N) is the Nth value of the sodium ion potential

ZNL(L,N) is the Nth value of the potential for the Lth wave function

PROGRAM FORM:

A. Type of Code FORTRAN 7090

B. Type of Monitor BELL

C. Number of Tape Units required (other than System Tapes): None

CODING INFORMATION:

A. Storage Required

1. Regular: 3894 (Total)

2. Common: 19037 (Total)

B. Accuracy:

TE – The accuracy to which the eigenvalues are to be calculated can be prescribed.

TT – The sum of squared deviations of iterated wave functions can be prescribed.

C. Timing:

It takes about 7 minutes to calculate 70 values for each of the three wave functions, when the prescribed accuracy of the eigenvalues is TE = 10^{-3} and the prescribed sum of squared deviations of iterated wave functions is TT = 10^{-2} .

D. Additional Subroutines Required:

This program uses only subroutines on the library tape and subroutines incorporated in this program. In fact this program has been split into the following subroutines:

1) Main Hartree Storage 217 + Common is the Main program.

2) Subroutine BINT(L) Storage 304 + Common. It calculates the Lth wave function by integrating backwards from large r values to small ones .

3) Subroutine EIGEN(L) Storage 283 + Common. It determines the Lth eigenvalue.

4) Subroutine FINT(L) Storage 390 + Common. It calculates the Lth wave function by integrating forward.

5) Subroutine OUTPUT Storage 182 + Common. Prints the final results.

6) Subroutine PRINT(L) Storage 41 + Common. Prints for the Lth wave function the values obtained by forward integration as well as the values obtained by backward integration. It also prints the Lth eigenvalue.

7) Subroutine RADIUS Storage 59 + Common. Divides the r-range into several sets and covers each of these sets by equidistant points.

8) Subroutine RINT(U) Storage 137 + Common. Dimension U(1000) calculates the integral of a function defined on the points calculated in Radius. U are the values of the integral, the function itself is transmitted through Common.

9) Subroutine SSRI(L) Storage 244 + Common. Calculates certain integrals of the Lth wave function

10) Subroutine TEST Storage 153 + Common. Tests whether the calculated wave functions fulfill the required accuracy.

11) Function YB(A,D,L) Storage 128 + Common
Dimension A(10), D(2)
Is a backward interpolation for A, to get from one set of equidistant r-values into the preceding one.

12) Function YF(A,D,I) Storage 81 + Common.
Dimension A(7), D(2)
Is a forward interpolation for A, to get from one set of equidistant r-values into the following one.

13) Subroutine Y2(P2) Storage 1088 + Common

Dimension P2(1000)

Calculates some integrals of the wave functions.

14) Subroutine ZPI Storage 101 + Common. Calculates the potentials for the wave functions.

USE:

The determination of these wave functions was undertaken in connection with a sodium-arc-tunnel project. With their aid cross-sections, transition-probabilities, line strength and line profiles can be calculated. This in turn can be used for interpretation of experimental data.

SPECIAL FEATURES: None

RESTRICTIONS:

A. Error Comments and Stops:

The program calls ENDJOB if

a) NFF > 1000 where NFF is the number of values of a single wave function.

b) NF(JS(L)) < 6 where NF(JS(L)) is the number of equidistant points in the r-range in which the forward and backward integrated solution of the Lth wave function are matched.

B. Range of Parameters:

a) NFF $\leq$ 1000 where NFF is the number of points of a single wave function.

b) JF $\leq$ 20 JF is the number of sets into which the r-range is divided. Each of these ranges is again subdivided into equal intervals.

APPENDIX A

Listing of Program

```
      FOR
C     MAIN HARTREE
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
     1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
   10 READ 1000,JF
   20 READ 1001,(NF(J),XF(J),J=1,JF)
   21 READ 1003,(JS(L),L=1,3)
   22 DO 28 L=1,3
   23 JSS=JS(L)
   24 IF(6-NF(JSS))25,25,180
   25 IS(L)=1+NF(JSS)/2
   26 JS1=JSS-1
   27 DO 28 J=1,JS1
   28 IS(L)=IS(L)+NF(J)
   30 NFF=1
   40 DO 50 J=1,JF
   50 NFF=NFF+NF(J)
   60 IF(NFF-1000) 70,70,180
   70 READ 1002,TE,TT,E(1),E(2),E(3),((P(L,N),L=1,3),N=1,NFF)
   80 CALL RADIUS
   90 DO 120 L=1,3
  100 CALL SSRL(L)
  105 X= SQRTF(S(L,NFF))
  110 DO 120 N=1,NFF
  120 P(L,N)=P(L,N)/X
  130 CALL TEST
  140 CALL ZPI
  150 DO 160 L=1,3
  160 CALL EIGEN(L)
  170 GO TO 90
 1000 FORMAT (I3)
 1001 FORMAT (I4,E14.6)
 1002 FORMAT (5E14.6/(3E14.6))
 1003 FORMAT (3I3)
  180 CALL SYSTEM
      END
```

```
      FOR
     SUBROUTINE BINT(L)
     COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
     DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
    1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
  20 B=.000000001
  30 W=DX(JF)**2/12.
  40 C=(ZNL(L,NFF-1)+E(L))*DX(JF)**2
  50 X=C/2.+SQRTF(C*(1.+C/2.))
  60 PB(NFF)=B/(1.+X)
  70 PB(NFF-1)=B
  80 NA=NFF
  90 JA=JF-JS(L)+1
 100 DO 190 K=1,JA
 110 J=JF+1-K
 120 NF1=NF(J)-1
 130 DO 150 M=1,NF1
 140 N=NA-1-M
 150 PB(N)=(PB(N+1)*(2.+W*(ZNL(L,N+1)+E(L))*10.
    1                                       )+PB(N+2)*(W*(ZNL(L,N+2)+E(
    2L))-1.))/(1.-W*(ZNL(L,N)+E(L)))
 160 NA=NA-NF(J)
 170 M=NA-1
 180 W=DX(J-1)**2/12.
 190 PB(M)=(PB(M+1)*(2.+W*(ZNL(L,M+1)+E(L))*10.
    1                                       )+YF(PB(M+1),DX(J-1),1)*(W*
    2(YF(ZNL(L,M+1),DX(J-1),3)+E(L))-1.))/(1.-W*(ZNL(L,M)+E(L)))
     RETURN
      END
```

```
      FOR
      SUBROUTINE EIGEN(L)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
     1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
   10 CALL FINT(L)
   20 EL=E(L)
   30 AL=P(L,NFF)
   40 E(L)=EL+.001
   50 CALL FINT(L)
   60 IF(SIGNF(1.,AL)*P(L,NFF)) 70,70,110
   70 EU=EL
   80 AU=AL
   90 GO TO 210
  110 IF(P(L,NFF)) 120,280,130
  120 IF(AL-P(L,NFF)) 20,20,140
  130 IF(AL-P(L,NFF)) 140,20,20
  140 E(L)=EL-.001
  150 GO TO 50
  160 EO=E(L)
  170 E(L)=(AU*EL-AL*EU)/(AU-AL)
  180 DE =ABSF(EO-E(L))
  190 IF(DE-TE) 280,200,200
  200 CALL FINT(L)
  210 IF(P(L,NFF)) 220,280,250
  220 AL=P(L,NFF)
  230 EL=E(L)
  240 GO TO 160
  250 AU=P(L,NFF)
  260 EU=E(L)
  270 GO TO 160
  280 CALL BINT(L)
  290 ISS=IS(L)
  300 X=P(L,ISS)/PB(ISS)
  310 DO 320 N=ISS,NFF
  320 P(L,N)=PB(N)*X
  330 CALL SSRL(L)
  340 W=SQRTF(S(L,NFF))
  350 DO 360 N=1,NFF
  360 P(L,N)=P(L,N)/W
  370 CALL ZPI
  380  CALL PRINT(L)
  390 IF(ABSF(A-E(L))-TE) 420,400,400
  400 A=E(L)
  410 GO TO 10
  420 RETURN
      END
```

```
     FOR
    SUBROUTINE FINT(L)
    COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
    DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
   1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
 10 FIRSTF(X)=X**(B+1.)*(1.-X    *11./(1.+B)+X    **2/(6.+4.*B)*((2.-B)*
   1121.-V)-11./(18.*(1.+B*9.))*((1.+B)*121.-(2.+5.*B)*V)*X    **3)
 20 B=FLOATF(L/3)
 30 W=DX(1)**2/12.
 40  V=4.*(RR(1,NFF)/S(1,NFF)+RR(2,NFF)/S(2,NFF)+3.*RR(3,NFF)/S(3,NFF)
   1)-2.*RR(L,NFF)/S(L,NFF)-E(L)
 60 P(L,1)=0.
 80 P(L,2)=FIRSTF(R(2))
100 P(L,3)=FIRSTF(R(3))
110 K=1
120 KA=3
130 DO 210 J=1,JF
140 M=K+KA
150 K=K+NF(J)
160 DO 170 N=M,K
170 P(L,N)=(P(L,N-1)*(2.+W*(ZNL(L,N-1)+E(L))*10.)+ P(L,N-2)*(W*(ZNL
   1(L,N-2)+E(L))-1.))/(1.-W*(ZNL(L,N)+E(L)))
180 IF(J-JF) 190,210,190
190 W=DX(J+1)**2/12.
200 P(L,K+1)=(P(L,K)*(2.+W*(ZNL(L,K)+E(L))*10.)+YB(P(L,K-3),DX(J),3)*(
   1W*(YB(ZNL(L,K-3),DX(J),3)+E(L))-1.))/(1.-W*(ZNL(L,K+1)+E(L)))
210 KA=2
220 RETURN
     END
```

```
      FOR
      SUBROUTINE OUTPUT
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
     1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000)
   10 READ 1000,D1,D2
   20 PRINT1001,D1,D2,E(1),E(2),E(3),TE,TT,R(1),P(1,1),P(2,1),P(3,1),
     1Z(1),ZNL(1,1),ZNL(2,1),ZNL(3,1)
   30 M=1
   40 DO 70 J=1,JF
   50 K=M+1
   60 M=M+NF(J)
   70 PRINT 1002,(R(N),P(1,N),P(2,N),P(3,N),Z(N),ZNL(1,N),ZNL(2,N),ZNL
     1(3,N),N=K,M)
   90 CALL ENDJOB
 1000 FORMAT (2A5)
 1001 FORMAT (1H1,36X,47HWAVE FUNCTIONS FOR SODIUM ION BY HARTREE METHOD
     1//55X,2A5////17X,3HE1=E14.9,17X,3HE2=E14.9,17X,3HE3=E14.9/
     2           25H  ACCURACY OF EIGENVALUE=E14.6,40X,26HACCURACY OF WA
     3VEFUNCTIONS=E14.6///3H  R13X,6HP1S(R),8X,6HP2S(R),8X,6HP2P(R),8X,4
     4HZ(R),11X,6HZ1S(R),8X,6HZ2S(R),8X,6HZ2P(R)//8E14.6)
 1002 FORMAT (1H /(8E14.6))
 1003 FORMAT (3E14.6)
      END
```

```
      FOR
     SUBROUTINE PRINT(L)
     COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
     DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
    1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
  10 PRINT 1000 ,(P(L,N),PB(N),N=1,NFF),E(L)
  20 RETURN
1000 FORMAT (2E18.9)
      END
```

```
      FOR
     SUBROUTINE RADIUS
     COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL
     DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
    1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000)
  10 K=1
  20 A=0.
  30 R(1)=0.
  40 DO 100 J=1,JF
  50 M=K+1
  60 K=K+NF(J)
  70 A=XF(J)-A
  80 DX(J)=A/FLOATF(NF(J))
     A=XF(J)
  90 DO 100 N=M,K
 100 R(N)=R(N-1)+DX(J)
 110 RETURN
      END
```

```
      FOR
      SUBROUTINE RINT(U)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
     1,X1
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
     1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
     2,U(1000),X1(1000)
      A=DX(1)/12.
      X1(1)=0.
       U(1)=0.
      U(2)=A*(8.*X1(2)-X1(3))
      K=1
      DO 30 J=1,JF
      M=K+2
      K=K+NF(J)
      DO 20 N=M,K
      B=-X1(N-2)
      C=8.*X1(N-1)
      D=5.*X1(N)
   20 U(N)=U(N-1)+A*(B+C+D)
      IF(J-JF) 25,30,35
   25 A=DX(J+1)/12.
      B=-YB(X1(K-3),DX(J),1)
      C=8.*X1(K)
      D=5.*X1(K+1)
      U(K+1)=U(K)+A*(B+C+D)
   30 CONTINUE
   35 RETURN
       END
```

```
      FOR
     $UBROUTINE SSRL(L)
     COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
     DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
    1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
  10 R(1)=1.
  30 S(L,1)=0.
  31 A=DX(1)/12.
  32 B=8.*P(L,2)**2
  33 C=-P(L,3)**2
  40 S(L,2)=A*(B+C)
  50 RR(L,1)=0.
  60 RR(L,2) = A*(B/R(2)+C/R(3))
  70 K=1
  80 DO 170 J=1,JF
  90 M=K+2
 100 K=K+NF(J)
 110 DO 130 N=M,K
 111 B=-P(L,N-2)**2
 112 C=8.*P(L,N-1)**2
 113 D=5.*P(L,N)**2
 120 S(L,N)=S(L,N-1)+A*(B+C+D)
 130 RR(L,N)=RR(L,N-1)+A*(B/R(N-2)+C/R(N-1)+D/R(N))
 140 IF(J-JF) 141,170,190
 141 A=DX(J+1) /12.
 142 B=-YB(P(L,K-3),DX(J),3)**2
 143 C=8.*P(L,K)**2
 144 D=5.*P(L,K+1)**2
 150 S(L,K+1)=S(L,K)+A*(B+C+D)
 160 RR(L,K+1)=RR(L,K)+A*(B/R(K-1)+C/R(K)+D/R(K+1))
 170 CONTINUE
 180 R(1)=0.
 190 RETURN
      END
```

```
      FOR
      SUBROUTINE TEST
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
     1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
   10 K=1
   20 T=0.
   30 DO 100 J=1,JF
   40 M=K+2
   50 K=K+NF(J)
   60 A=0.
   70 DO 80 N=M,K,2
   80 A=A+SQ  (N-2)+4.*SQ  (N-1)+SQ  (N)
   90 A=A+FLOATF(NF(J)-(NF(J)/2)*2)*(-SQ  (K-2)+8.*SQ  (K-1)+5.*SQ  (K))
     1/4.
  100 T=T+A*DX(J)/3.
  110 IF(T-TT) 120,120,130
  120 CALL OUTPUT
  130 DO 150 L=1,3
  140 DO 150 N=1,NFF
  150 PF(L,N)=(P(L,N)+PF(L,N))/2.
  160 RETURN
      END
```

```
     FOR
    FUNCTION YB(A,D,L)
    DIMENSION A(10),D(2)
 10 B=-D(2)
 20 B1= B + D(1)
 30 B2 = B1 + D(1)
 40 B3 = B2 + D(1)
 50 C=6.*D(1)**3
 60 YB=(B1*B2*(A(3*L+1)*B3-A(1)*B)+3.*B*B3*(A(L+1)*B1-A(2*L+1)*B2))/C
 70 RETURN
     END
```

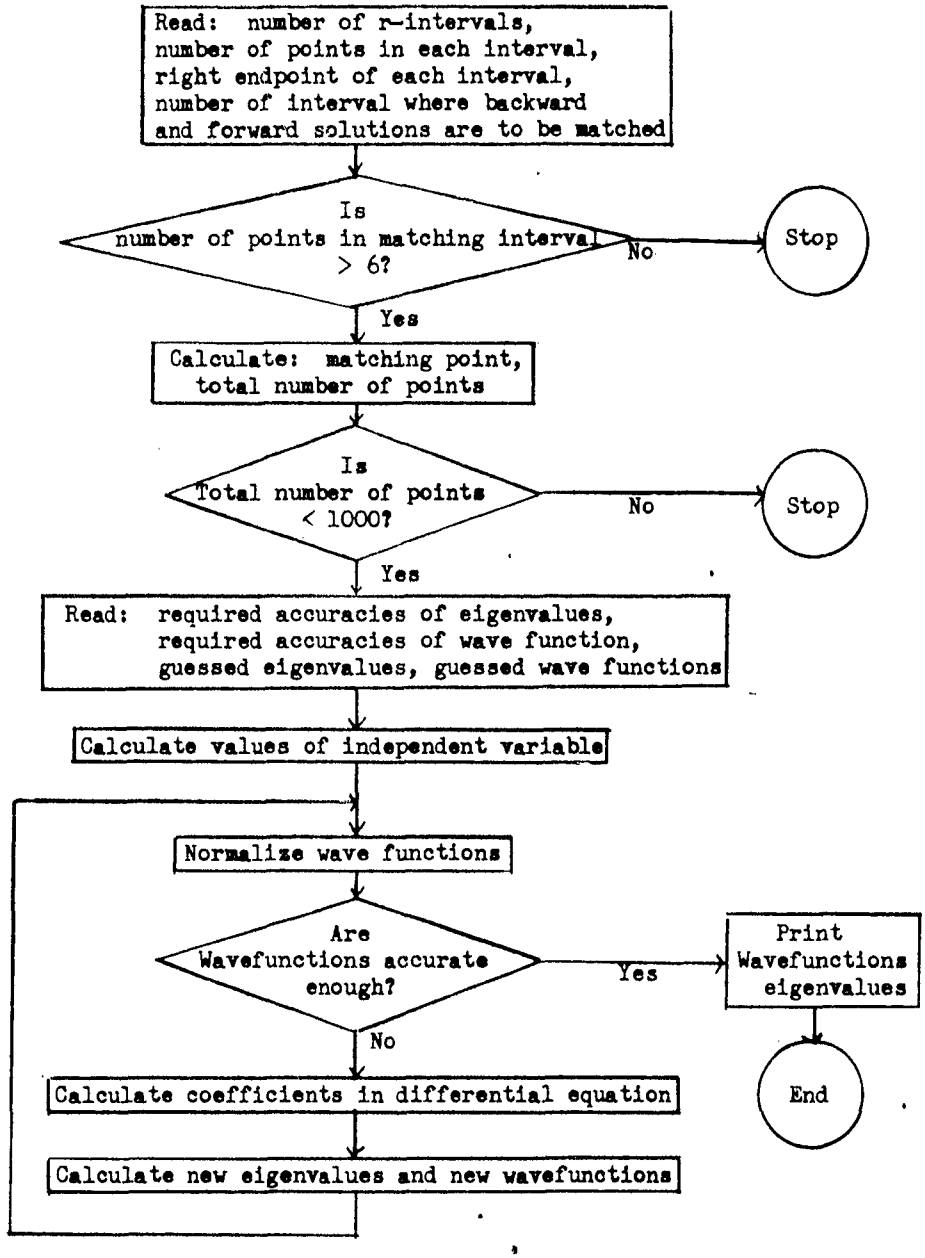
```
      FOR
     FUNCTION YF(A,D,L)
     DIMENSION A(7),D(2)
  10 B=A(2*L+1)-2.*A(L+1)+A(1)
  20 C=-A(2*L+1)+4.*A(L+1)-3.*A(1)
  30 X=D(1)/D(2)
  40 YF=(B*X+C)*X/2.+A(1)
  50 RETURN
      END
```

```
      SUBROUTINE Y2(P2)
      COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
     1,X1
      DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
     1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
     2,P2(1000),X1(1000),U(1000)
      DO 10 N=2,NFF
   10 X1(N)=(P(3,N)*R(N))**2
      CALL RINT(U)
      DO 20 N=2,NFF
   20 X1(N)=P(3,N)**2/R(N)**3
      CALL RINT(P2)
      P2(1)=0.
      DO 30 N=2,NFF
      H=R(N)**2
   30 P2(N)=U(N)/H+H*R(N)*(P2(NFF)-P2(N))
      RETURN
       END
```

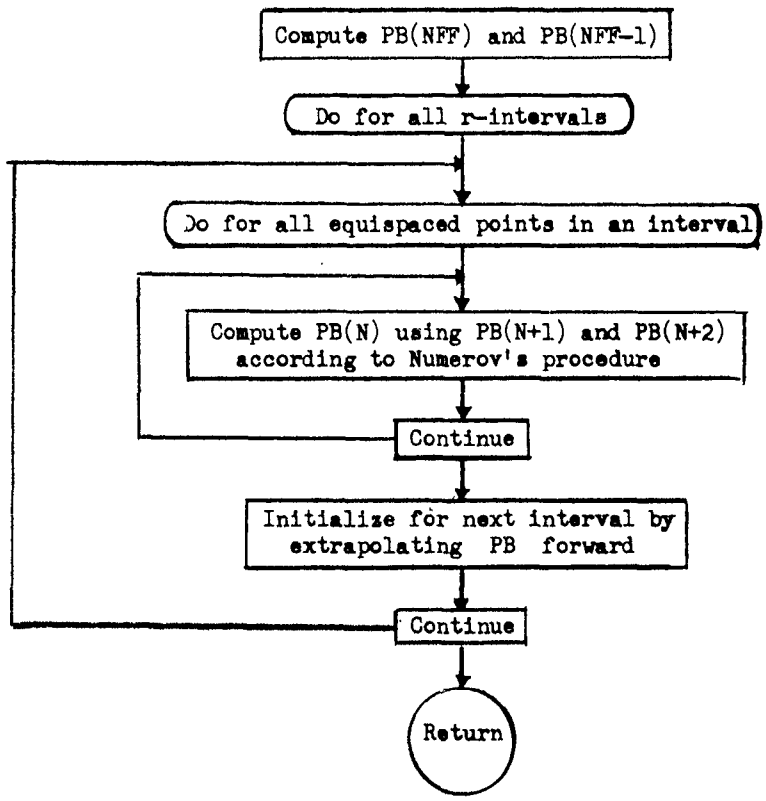
```
    FOR
   SUBROUTINE ZPI
   COMMON JF,NF,XF,DX,NFF,TE,TT,E,P,PF,R,S,RR,Z,ZNL,PB,JS,IS
   DIMENSION NF(20),XF(20),DX(20),E(3),P(3,1000),PF(3,1000),R(1000),
  1S(3,1000),RR(3,1000),Z(1000),ZNL(3,1000),PB(1000),JS(3),IS(3)
10 R(1)=1.
   CALL Y2(Z)
30 DO 70 N=2,NFF
31 A=Y(1,N)
32 B=Y(2,N)
33 C=Y(3,N)
40 EE  =-11.+2.*(A+B+3.*C)
41 D=2./R(N)
50 ZNL(1,N)=D*(EE  -A)
60 ZNL(2,N)=D*(EE  -B)
70 ZNL(3,N)=D*(EE  -C-.4*Z (N)+1./R(N))
80 R(1)=0.
90 RETURN
    END
```

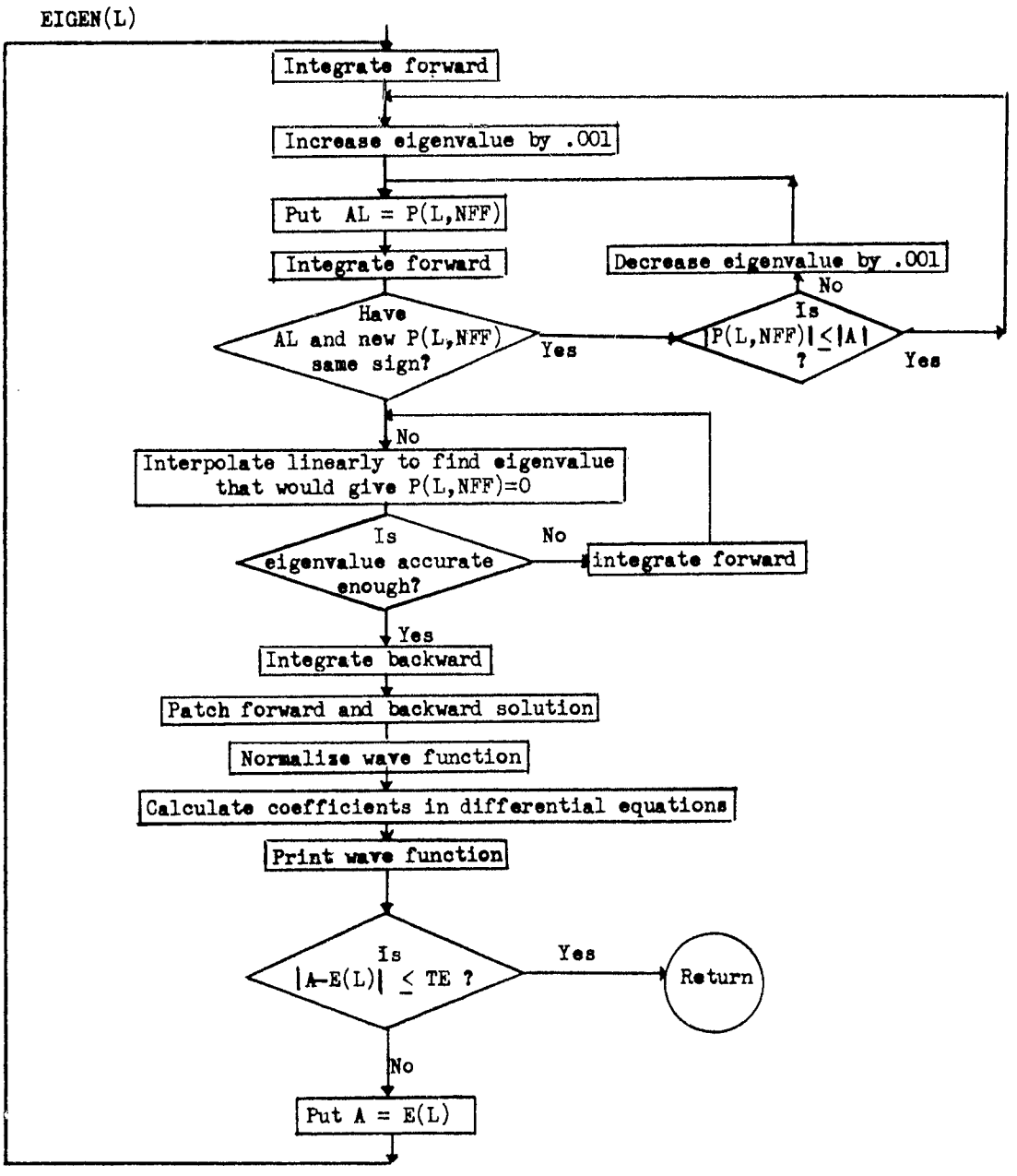
APPENDIX B – FLOW CHART

MAIN ROUTINE

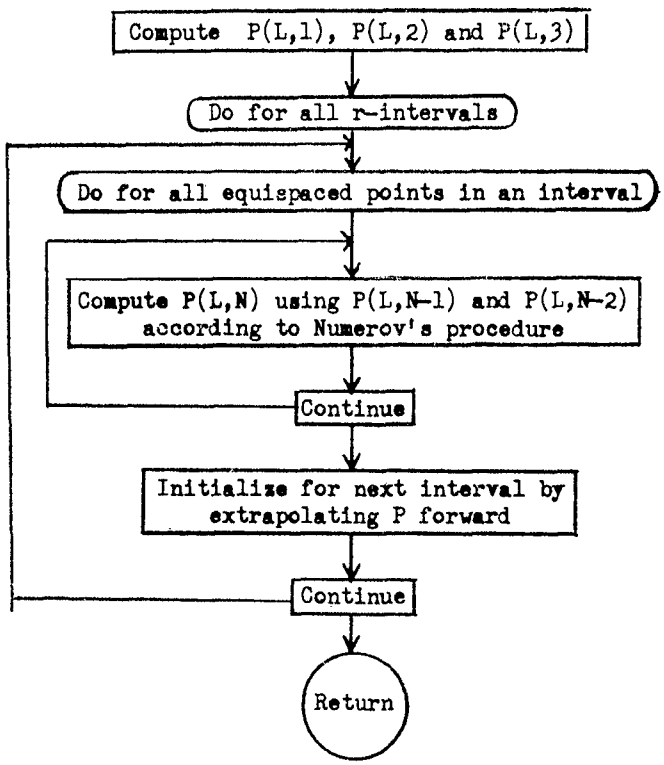


BINT(L)

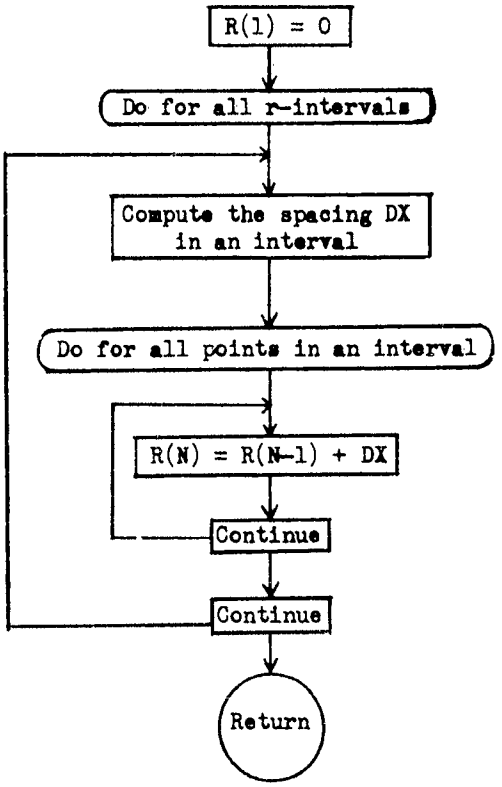

Compute PB(NFF) and PB(NFF-1)
Do for all r-intervals
Do for all equispaced points in an interval
Compute PB(N) using PB(N+1) and PB(N+2) according to Numerov's procedure
Continue
Initialize for next interval by extrapolating PB forward
Continue
Return


EIGEN(L)
Integrate forward
Increase eigenvalue by .001
Put AL = P(L,NFF)
Integrate forward
Have AL and new P(L,NFF) same sign?
Yes
Is |P(L,NFF)| ≤ |A| ?
No
Yes
Decrease eigenvalue by .001
No
Interpolate linearly to find eigenvalue that would give P(L,NFF)=0
Is eigenvalue accurate enough?
No
Integrate forward
Yes
Integrate backward
Patch forward and backward solution
Normalize wave function
Calculate coefficients in differential equations
Print wave function
Is |A-E(L)| ≤ TE ?
Yes
Return
No
Put A = E(L)

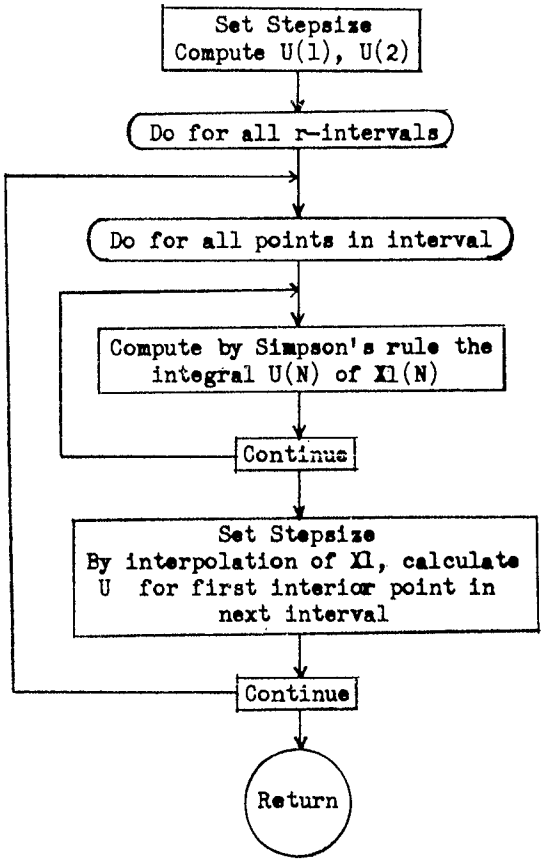
FINT(L)


Compute P(L,1), P(L,2) and P(L,3)
Do for all r-intervals
Do for all equispaced points in an interval
Compute P(L,N) using P(L,N-1) and P(L,N-2) according to Numerov's procedure
Continue
Initialize for next interval by extrapolating P forward
Continue
Return

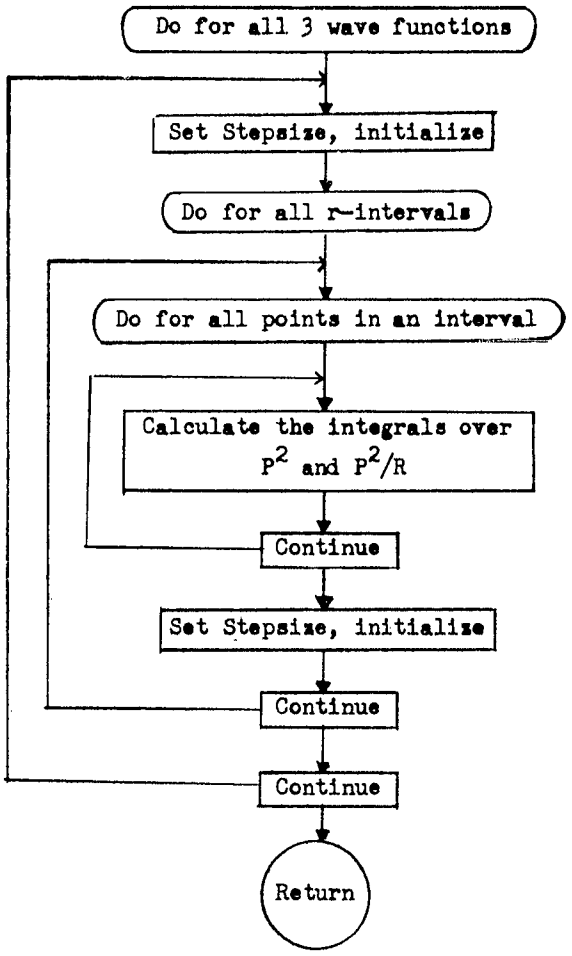
RADIUS


R(1) = 0
Do for all r-intervals
Compute the spacing DX in an interval
Do for all points in an interval
R(N) = R(N-1) + DX
Continue
Continue
Return

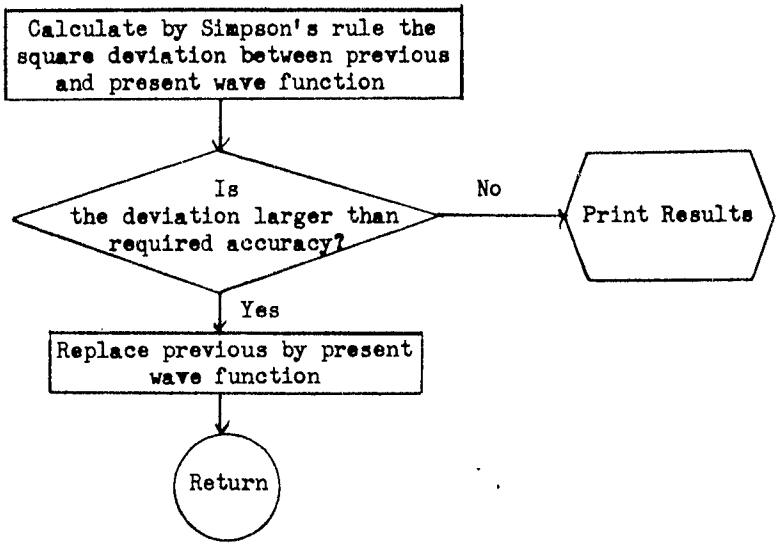
RINT(U)


Set Stepsize
Compute U(1), U(2)
Do for all r-intervals
Do for all points in interval
Compute by Simpson's rule the integral U(N) of X1(N)
Continue
Set Stepsize
By interpolation of X1, calculate U for first interior point in next interval
Continue
Return

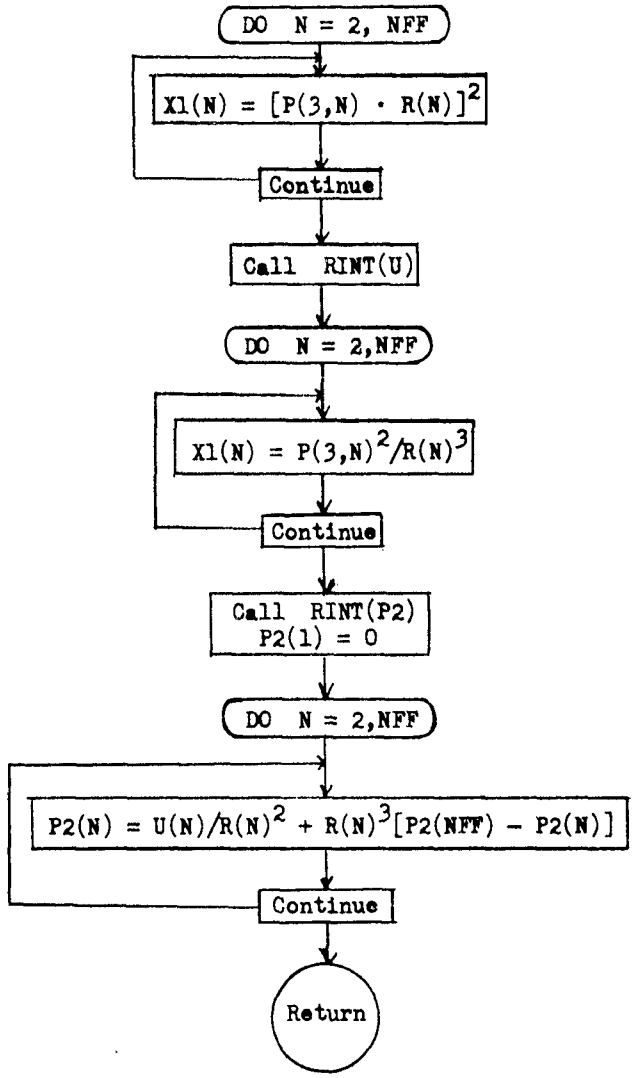
SSR


Do for all 3 wave functions
Set Stepsize, initialize
Do for all r-intervals
Do for all points in an interval
Calculate the integrals over P^2 and P^2/R
Continue
Set Stepsize, initialize
Continue
Continue
Return

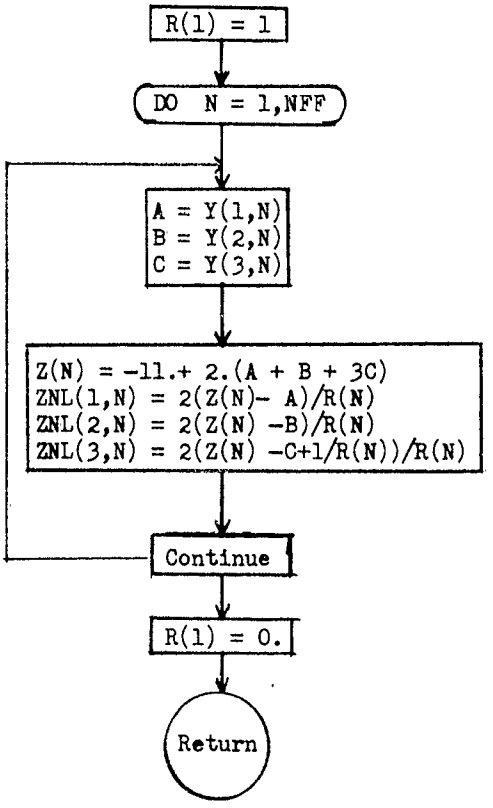
TEST


Calculate by Simpson's rule the square deviation between previous and present wave function
Is the deviation larger than required accuracy?
No
Print Results
Yes
Replace previous by present wave function
Return

Y2(P2)


DO N = 2, NFF
X1(N) = [P(3,N) · R(N)]^2
Continue
Call RINT(U)
DO N = 2,NFF
X1(N) = P(3,N)^2/R(N)^3
Continue
Call RINT(P2)
P2(1) = 0
DO N = 2,NFF
P2(N) = U(N)/R(N)^2 + R(N)^3[P2(NFF) - P2(N)]
Continue
Return

ZPI


R(1) = 1
DO N = 1,NFF
A = Y(1,N)
B = Y(2,N)
C = Y(3,N)
Z(N) = -11.+ 2.(A + B + 3C)
ZNL(1,N) = 2(Z(N)- A)/R(N)
ZNL(2,N) = 2(Z(N) -B)/R(N)
ZNL(3,N) = 2(Z(N) -C+1/R(N))/R(N)
Continue
R(1) = 0.
Return

APPENDIX C

EXAMPLE:

The r-range was chosen from 0 to 10.

It was divided into 5 sets, so JF = 5.

These sets were

from 0	to 0.04	0.01	so NF(1) = 4 ,	XF(1) = .04
0.04	0.2	0.02	NF(2) = 8 ,	XF(2) = .2
0.2	0.5	0.05	NF(3) = 6 ,	XF(3) = .5
0.5	1.2	0.1	NF(4) = 7 ,	XF(4) =1.2
1.2	10	0.2	NF(5) = 44,	XF(5) =10.

the forward and backward integrated solutions get matched in the interval

$0.5 \leq r \leq 1.2$ so

JS(1) = 4 JS(2) = 4 JS(3) = 4

The permissible absolute error for the eigenvalues was chosen to be 10^{-4}

so $TE = 10^{-4}$.

The permissible sum of squared deviations of wave functions was chosen to be 10^{-3}

so $TT = 10^{-3}$.

The guesses for the 3 eigenvalues were taken as

E(1) = 81 E(2) = 4.546948 E(3) = 3.204463

Since $NFF = 1 + \sum_{j=1}^{5} NF(J) = 70$ there follows three columns with 70 values each for the guesses of the three wave functions.

The last input is the DATE 01-25-1962

```
     TRA
5
 4    .04
 8    .2
 6    .5
 7   1.2
44  10.
 4   4   4
  .1      E-03    .1      E-02 81.            4.546948       3.204463
-0.             -0.             -0.
 0.629350E 00    0.154058E-00    0.400036E-02
 0.112863E 01    0.274103E-00    0.140013E-01
 0.151784E 01    0.366138E-00    0.300027E-01
 0.181501E 01    0.433163E-00    0.500045E-01
 0.219322E 01    0.507191E 00    0.102009E-00
 0.235731E 01    0.517195E 00    0.163015E-00
 0.237832E 01    0.481181E-00    0.231021E-00
 0.230628E 01    0.412155E-00    0.302027E-00
 0.217621E 01    0.320121E-00    0.374034E-00
 0.201312E 01    0.215081E-00    0.444040E-00
 0.183502E 01    0.102038E-00    0.512046E 00
 0.165292E 01   -0.150057E-01    0.578052E 00
 0.122768E 01   -0.301114E-00    0.724065E 00
 0.878488E 00   -0.555209E 00    0.842076E 00
 0.614341E 00   -0.763288E 00    0.933084E 00
 0.422235E-00   -0.923348E 00    0.997090E 00
 0.287160E-00   -0.103739E 01    0.103909E 01
 0.194108E-00   -0.111242E 01    0.106110E 01
 0.880489E-01   -0.116944E 01    0.106110E 01
 0.400222E-01   -0.113943E 01    0.102109E 01
 0.180100E-01   -0.106140E 01    0.956086E 00
 0.800445E-02   -0.958361E 00    0.880079E 00
 0.300167E-02   -0.846319E 00    0.799072E 00
 0.100056E-02   -0.736278E 00    0.718065E 00
-0.             -0.632238E 00    0.640058E 00
-0.             -0.455172E-00    0.501045E 00
-0.             -0.319120E-00    0.385035E-00
-0.             -0.220083E-00    0.292026E-00
-0.             -0.149056E-00    0.219020E-00
-0.             -0.101038E-00    0.163015E-00
-0.             -0.680257E-01    0.121011E-00
-0.             -0.450170E-01    0.890080E-01
-0.             -0.300113E-01    0.650058E-01
-0.             -0.200075E-01    0.480043E-01
-0.             -0.130049E-01    0.350031E-01
-0.             -0.900340E-02    0.260023E-01
-0.             -0.600226E-02    0.190017E-01
-0.             -0.400151E-02    0.140013E-01
-0.             -0.200075E-02    0.100009E-01
-0.             -0.914625E-03    0.691489E-02
 0.             -0.120045E-02    0.488044E-02
-0.             -0.800305E-03    0.328030E-02
 0.             -0.280106E-03    0.268024E-02
 0.             -0.596273E-10    0.200018E-02
-0.              0.              0.148013E-02
 0.              0.              0.120011E-02
-0.             -0.              0.800072E-03
 0.              0.              0.280025E-03
 0.              0.              0.119220E-09
 0.              0.              0.
```

-0.	-0.	-0.
0.	0.	0.
0.	0.	0.
-0.	-0.	-0.
0.	0.	0.
-0.	-0.	-0.
0.	0.	0.
0.	0.	0.
-0.	-0.	0.

01-25-1963

EXAMPLE (OUTPUT)

WAVE FUNCTIONS FOR SODIUM ION BY HARTREE METHOD

01-25-1962

E1=.3818864136 02 E2=.4754947426 01 E3=.3252275966 01

ACCURACY OF EIGENVALUE= 1.0000000E-04 ACCURACY OF WAVEFUNCTIONS= 1.0000000E-03

R	P1S(R)	P2S(R)	P2P(R)	Z(R)	Z1S(R)	Z2S(R)	Z2P(R)
0.	0.	0.	0.	0.	0.	0.	0.
1.0000000E-02	0.639562E 00	0.159695E-06	0.352282E-12	0.155083E-04	-0.215144E 04	-0.213362E 04	0.178666E 03
0.2000000E-01	0.114035E 01	0.267309E-06	0.132956E-11	0.127351E-03	-0.105192E 04	-0.103452E 04	0.396569E 03
0.3000000E-01	0.153023E 01	0.356338E-06	0.265970E-11	0.424786E-03	-0.685691E 03	-0.669026E 03	0.155337E 03
0.4000000E-01	0.182744E 01	0.421653E-06	0.478404E-11	0.990840E-03	-0.503302E 03	-0.487071E 03	0.763061E 02
0.6000000E-01	0.220834E 01	0.494053E-06	0.971936E-11	0.321902E-02	-0.321755E 03	-0.307046E 03	0.248532E 02
0.8000000E-01	0.236337E 01	0.506283E 06	0.156426E-10	0.725342E-02	-0.231822E 03	-0.218592E 03	0.938227E 01
1.0000000E-01	0.238427E 01	0.474884E-06	0.221856E-10	0.133731E-01	-0.173482E 03	-0.166668E 03	0.331424E 01
0.1200000E-00	0.236965E 01	0.412486E-06	0.290470E-10	0.216986E-01	-0.143349E 03	-0.132842E 03	0.576103E 01
0.1400000E-00	0.217736E 01	0.326768E-06	0.360223E-10	0.322185E-01	-0.118550E 03	-0.109221E 03	-0.755209E 01
0.1600000E-00	0.201251E 01	0.231170E-06	0.429392E-10	0.448175E-01	-0.100155E 03	-0.918781E 02	-0.141983E 02
0.1800000E-00	0.183249E 01	0.125404E-06	0.496707E-10	0.593046E-01	-0.859960E 02	-0.786477E 02	-0.174267E 02
0.2000000E-00	0.164912E 01	0.158450E-01	0.561227E-10	0.754371E-01	-0.747774E 02	-0.682472E 02	-0.188058E 02
0.2500000E-00	0.122620E 01	-0.254643E-06	0.706347E-10	0.121177E-00	-0.549188E 02	-0.500484E 02	-0.186907E 02
0.3000000E-00	0.869475E 00	-0.493215E-06	0.824612E-10	0.170974E-00	-0.419658E 02	-0.382803E 02	-0.167398E 02
0.3500000E-00	0.604112E 00	-0.720673E 06	0.915265E-10	0.220982E-00	-0.329722E 02	-0.301619E 02	-0.145258E 02
0.4000000E-00	0.412280E-00	-0.859067E 06	0.980260E-10	0.268228E-00	-0.264558E 02	-0.242994E 02	-0.124786E 02
0.4500000E-00	0.277699E-00	-0.973689E 06	0.102265E-09	0.310697E-00	-0.215933E 02	-0.199306E 02	-0.107098E 02
0.5000000E-00	0.185228E-00	-0.105536E 01	0.104598E-09	0.347223E-00	-0.178863E 02	-0.165997E 02	-0.922489E 01
0.6000000E 00	0.806478E-01	-0.112668E 01	0.104830E-09	0.401643E-00	-0.127978E 02	-0.120155E 02	-0.701710E 01
0.7000000E 00	0.344518E-01	-0.111537E 01	0.101163E-09	0.432342E-00	-0.957049E 01	-0.909203E 01	-0.549981E 01
0.8000000E 00	0.145029E-01	-0.105482E 01	0.951252E-10	0.443334E-00	-0.745716E 01	-0.716278E 01	-0.446410E 01
0.9000000E 00	0.609100E-02	-0.968093E 00	0.878930E-10	0.439473E-00	-0.602637E 01	-0.584437E 01	-0.374489E 01
1.0000000E 00	0.255303E-02	-0.876342E 00	0.802052E-10	0.425243E-00	-0.502710E 01	-0.491412E 01	-0.323378E 01
0.1100000E 01	0.105398E-02	-0.770889E 00	0.725174E-10	0.404301E-00	-0.430797E 01	-0.423758E 01	-0.286065E 01
0.1200000E 01	0.451309E-03	-0.675220E 00	0.651039E-10	0.379428E-00	-0.377510E 01	-0.373111E 01	-0.258621E 01
0.1400000E 01	0.740344E-04	-0.505907E 00	0.516722E-10	0.329955E-00	-0.305960E 01	-0.304121E 01	-0.220013E 01
0.1600000E 01	0.120685E-04	-0.370480E-00	0.403755E-10	0.281585E-00	-0.259095E 01	-0.258359E 01	-0.193778E 01
0.1800000E 01	0.195765E-05	-0.266977E-00	0.311857E-10	0.238547E-00	-0.226361E 01	-0.226065E 01	-0.174644E 01
0.2000000E 01	0.316485E-06	-0.190087E-00	0.238699E-10	0.201997E-00	-0.201903E 01	-0.201784E 01	-0.159706E 01
0.2200000E 01	0.510525E-07	-0.134069E-00	0.181350E-10	0.171679E-00	-0.182701E 01	-0.182653E 01	-0.147491E 01
0.2400000E 01	0.821181E-08	-0.938365E-01	0.136921E-10	0.146793E-00	-0.167079E 01	-0.167060E 01	-0.137188E 01
0.2600000E 01	0.131913E-08	-0.652597E-01	0.102823E-10	0.126423E-00	-0.154604E 01	-0.154632E 01	-0.128315E 01
0.2800000E 01	0.211595E-09	-0.451409E-01	0.768568E-11	0.109717E-00	-0.142949E 01	-0.142946E 01	-0.120559E 01
0.3000000E 01	0.338989E-10	-0.310796E-01	0.572123E-11	0.959470E-01	-0.133377E 01	-0.133376E 01	-0.113706E 01
0.3200000E 01	0.542498E-11	-0.213120E-01	0.424337E-11	0.845183E-01	-0.125021E 01	-0.125020E 01	-0.107599E 01
0.3400000E 01	0.867539E-12	-0.145623E-01	0.313702E-11	0.749615E-01	-0.117657E 01	-0.117657E 01	-0.102118E 01
0.3600000E 01	0.138559E-12	-0.991899E-02	0.231232E-11	0.669095E-01	-0.111116E 01	-0.111116E 01	-0.971700E 00
0.3800000E 01	0.221181E-13	-0.673730E-02	0.169991E-11	0.600761E-01	-0.105266E 01	-0.105266E 01	-0.926795E 00
0.4000000E 01	0.352632E-14	-0.456468E-02	0.124668E-11	0.542390E-01	-0.100001E 01	-0.100001E 01	-0.885858E 00
0.4200000E 01	0.562504E-15	-0.308565E-02	0.912284E-12	0.492043E-01	-0.952387E 00	-0.952387E 00	-0.848380E 00
0.4400000E 01	0.896281E-16	-0.208154E-02	0.666234E-12	0.448446E-01	-0.909094E 00	-0.909094E 00	-0.813942E 00
0.4600000E 01	0.142740E-16	-0.140155E-02	0.485642E-12	0.410360E-01	-0.869567E 00	-0.869567E 00	-0.782186E 00
0.4800000E 01	0.227220E-17	-0.942067E-03	0.353395E-12	0.376909E-01	-0.833335E 00	-0.833335E 00	-0.752811E 00

0.500000E 01	0.361548E-18	-0.632221E-03	0.256753E-02	0.347377E-01	-0.800001E 00	-0.800001E 00	-0.725559E 00
0.520000E 01	0.575065E-19	-0.423665E-03	0.186265E-02	0.321179E-01	-0.769231E 00	-0.769231E 00	-0.700208E 00
0.540000E 01	0.914349E-20	-0.283525E-03	0.134943E-02	0.297833E-01	-0.740741E 00	-0.740741E 00	-0.676566E 00
0.560000E 01	0.145332E-20	-0.189503E-03	0.976363E-03	0.276942E-01	-0.714286E 00	-0.714286E 00	-0.654467E 00
0.580000E 01	0.230928E-21	-0.126513E-03	0.705590E-03	0.258173E-01	-0.689655E 00	-0.689655E 00	-0.633763E 00
0.600000E 01	0.366832E-22	-0.843693E-04	0.509338E-03	0.241249E-01	-0.666667E 00	-0.666667E 00	-0.614328E 00
0.620000E 01	0.582560E-23	-0.562073E-04	0.367284E-03	0.225936E-01	-0.645161E 00	-0.645161E 00	-0.596048E 00
0.640000E 01	0.924919E-24	-0.374101E-04	0.264585E-03	0.212036E-01	-0.625000E 00	-0.625000E 00	-0.578822E 00
0.660000E 01	0.146813E-24	-0.248770E-04	0.190424E-03	0.199380E-01	-0.606061E 00	-0.606061E 00	-0.562564E 00
0.680000E 01	0.232985E-25	-0.165289E-04	0.136929E-03	0.187824E-01	-0.588235E 00	-0.588235E 00	-0.547192E 00
0.700000E 01	0.369637E-26	-0.109735E-04	0.983795E-04	0.177245E-01	-0.571429E 00	-0.571429E 00	-0.532638E 00
0.720000E 01	0.586388E-27	-0.727988E-05	0.706269E-04	0.167535E-01	-0.555556E 00	-0.555556E 00	-0.518837E 00
0.740000E 01	0.930613E-28	-0.482610E-05	0.506631E-04	0.158601E-01	-0.540541E 00	-0.540541E 00	-0.505732E 00
0.760000E 01	0.147474E-28	-0.319727E-05	0.363173E-04	0.150363E-01	-0.526316E 00	-0.526316E 00	-0.493273E-00
0.780000E 01	0.233614E-29	-0.211684E-05	0.260178E-04	0.142751E-01	-0.512821E 00	-0.512821E 00	-0.481412E-00
0.800000E 01	0.370642E-30	-0.140066E-05	0.186261E-04	0.135703E-01	-0.500000E 00	-0.500000E 00	-0.470107E-00
0.820000E 01	0.587453E-31	-0.926260E-06	0.133262E-04	0.129164E-01	-0.487805E-00	-0.487805E-00	-0.459321E-00
0.840000E 01	0.930955E-32	-0.612203E-06	0.952870E-05	0.123087E-01	-0.476191E-00	-0.476191E-00	-0.449018E-00
0.860000E 01	0.147511E-32	-0.404416E-06	0.680949E-05	0.117428E-01	-0.465116E-00	-0.465116E-00	-0.439167E-00
0.880000E 01	0.233702E-33	-0.267023E-06	0.486361E-05	0.112151E-01	-0.454545E-00	-0.454545E-00	-0.429739E-00
0.900000E 01	0.370209E-34	-0.176219E-06	0.347193E-05	0.107222E-01	-0.444444E-00	-0.444444E-00	-0.420706E-00
0.920000E 01	0.586380E-35	-0.116236E-06	0.247718E-05	0.102611E-01	-0.434783E-00	-0.434783E-00	-0.412045E-00
0.940000E 01	0.928671E-36	-0.766303E-07	0.176648E-05	0.982910E-02	-0.425532E-00	-0.425532E-00	-0.403734E-00
0.960000E 01	0.147073E-36	-0.504871E-07	0.125896E-05	0.942382E-02	-0.416667E-00	-0.416667E-00	-0.395751E-00
0.980000E 01	0.	-0.332321E-07	0.896650E-06	0.904310E-02	-0.408163E-00	-0.408163E-00	-0.388077E-00
1.000000E 01	0.	-0.218393E-07	0.638039E-06	0.868500E-02	-0.400000E-00	-0.400000E-00	-0.380695E-00

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5. Hartree-Fock equations

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